DEPARTAMENT DE QUÍMICA FÍSICA 2026-2027

NÚMERO	TEMA	TUTOR(S) ACADÈMIC(S) (si un és d'un altre departament, posa'l entre parèntesi)	TUTOR EXTERN (si escau)
1	Computational Design of Ti-Metal–Organic Frameworks for Selective CO_2 Capture	Neyvis Almora Barrios/(Alechania Misturini Morelli)(Q.Inorgánica)	
2	Tuning Electronic and Optical Properties of Heterometallic Titanium Clusters Using Computational Tools	Neyvis Almora Barrios/(Alechania Misturini Morelli)(Q.Inorgánica)	
3	Theoretical study of the photophysics of Ru(II) transition metal complexes for photoinduced anticancer therapy	Antonio Fránces Monerris	
4	Syntesis and Characterization of New Iron(II) Spin Crossover Coordination Polymers	Carlos Bartual Murgui/Teresa Delgado Pérez	
5	Spin-crossover complexes as innovative contrast agents for magnetic resonance imaging (MRI)	Teresa Delgado Pérez/Carlos Bartual Murgui	
6	Exotic and emerging applications of persistent luminescence materials	Teresa Delgado Pérez	
7	Study of the selective oxidation over vanadia supported catalyst	Lourdes Gracia Edo	
8	Implementation of low-field NMR metabolomics for the determination of neurochemical brain alterations.	Mª Carmen Martínez Bisbal/Salvador Cardona Serra	
9	Thermogalvanic cells based on microfluidic circuits	Mario Culebras Rubio	
10	Lignin-based hydrogels for thermogalvanic cells	Mario Culebras Rubio	
11	Effect of seed layers on the photoluminescent efficiency of metal halide perovskites	Cristina Roldán Carmona	
12	Synthesis of thermoplastic polyurethanes with improved thermal resistance	Clara M. Gómez Clari	
13	Lignin/Cu2S Composites for Thermoelectric 3D-Printing Materials	Clara M. Gómez Clari/Mario Culebras Rubio	
14	Solar absorption spectra of atmospheric mercury compounds in water droplets	Daniel Roca Sanjuán/Antonio Francés Monerris	
15	Molecular basis of the chemiluminescence-induced photodynamic therapy	Daniel Roca Sanjuán/Antonio Francés Monerris	
16	Free energies of cations and anions of nucleobases in DNA: A computational study	Daniel Roca Sanjuán/Javier Segarra Martí	
17	Oxidation potential of DNA quadruplexes	Daniel Roca Sanjuán/Antonio Francés Monerris	
18	Validation of AI-predicted conformational ensembles of disordered peptides	Kirill Zinovjev	
19	Colloidal Encapsulation of High-Temperature Phase Change Materials	Rafael Muñoz-Espí / Mario Culebras Rubio	
20	A Computational Approach to the Study of Enzymatic Mechanisms.	Iñaki Tuñón / Jose Javier Ruíz	
21	Insights into the recognition of neurotransmitters by azamacrocycles: A theoretical approach.	Álvaro Martínez Camarena	
22	Design, Preparation and Catalytic Performance of Sustainable Nickel Nanoparticles Supported on Carbonized Polydopamine/magnetite cores.	Francisco F. Pérez Pla / Mª Ángles Úbeda Picot	
23	Application of Functionalized Polymer Nanoparticles in Asymmetric Catalysis	Rafael Muñoz-Espí /Francisco F. Pérez Pla	

24	Characterization of Enzyme Catalytic Properties Using Molecular Dynamics Simulations.	Jose Javier Ruiz/Iñaki Tuñón	
25	Transforming Biomass into Advanced Electrocatalyts:Pyrolyzed Lignin-Metal Electrodes for Green Aromatic Nitro Compound Reduction	Mario Culebras Rubio / Francisco F. Pérez Pla	
26	Polysaccharide-Based Hybrid Particles as Magnetically Separable Catalysts	Rafael Muñoz-Espí / Francisco F. Pérez Pla	
27	From Sustainable Materials to Efficient Catalysts:Preparation and Evaluation of Cobalt Nanoparticles on Carbonized Polydopamine/Co3O4 magnetic cores	Francisco F. Pérez Pla / Mª Ángles Úbeda Picot	
28	Color in the Chemistry Laboratory: Theoretical Foundations, Quantitative Rigor, and Instrumental Development.	José Juan García Jareñe / Jerónimo Agrisuelas Valles	
29	Microsolvation effects on the photophysical reactivity of DNA model systems	Javier Segarra Martí / Lewis Hutton	
30	Separation of cobalt and nickel metals by selective electrodeposition on different types of electrodes.	Jerónimo Agrisuelas Valles / José Juan García Jareño	
31	Mineralization of water pollutants by advanced oxidation techniques and spectroelectrochemical monitoring.	Jerónimo Agrisuelas Valles / José Juan García Jareño	
32	Generation of reactive oxygen species (ROS) on steel/poly(phenothiazines) electrodes and their application.	Jerónimo Agrisuelas Valles / José Juan García Jareño	
33	Electroplating of copper on composite materials of the screen printed carbon electrodes for their possible use in sensors.	Jerónimo Agrisuelas Valles / José Juan García Jareño	
34	Revisiting the absorption cross sections of atmospheric mercury compounds with anharmonic corrections and probabilistic machine learning	Daniel Roca Sanjuán /David Francisco Macias Pinilla	
35	Modelling the water UV/Vis spectrum: from gas phase to liquid	Javier Segarra Marti	
36	First-principles characterization of honeycomb 2D MOFs as porous conductors	Joaquín Calbo Roig / Enrique Ortí Guillén	
37	Development and Evaluation of Immersive Virtual Reality and Augmented Reality Modules for Teaching Stereochemistry, Crystal Structures, and Protein Architecture.	Jesús vicente de Julian Ortíz	Sofiane Benmetir
38	Design of Rotavirus Inhibitor Compounds	Jesús vicente de Julian Ortíz	Sofiane Benmetir
39	Computational Simulation of the T-lymphocyte receptor	Jesús vicente de Julian Ortíz	Sofiane Benmetir

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Neyvis Almora Barrios

ACADEMIC TUTOR 2 Alechania Misturini Morelli

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física / Química Inorgánica

TITLE (Mandatory in English)

Computational Design of Ti-Metal–Organic Frameworks for Selective CO_2 Capture

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

1. Identificar las aminas y la estabilidad de las redes metal-orgánicas de titanio (Ti-MOF) que potencialmente podrían interaccionar fuertemente entre si.

2. Estudiar la incorporación de las aminas en los Ti-MOFs a través de métodos de química computacional.

3. Estudiar la estabilidad termodinámica e identificar las interacciones directoras del sistema amina-Ti-MOFs.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. Revisión bibliográfica de las aminas usadas para capturar dióxido de carbono en MOFs.
2. Estudio conformacional de las moléculas seleccionadas en el paso 1, usando técnicas computacionales. Se usaran programas de visualización de estructuras tales como Materials Studio, vmd, gdis, and gview.
3. Estudio de estabilidad de Ti-MOFs. Se optimizaran las geometrías del los cristales con técnicas de campo de fuerza implementadas en códigos tal como GULP.
4. Calculo de la energía de interacción entre las aminas y los Ti-MOFs mas estables (segun el paso 2) usando métodos de Química Clásica.
5. Calcular la energía de adsorción del CO2 en los sistemas mas estables (identificados en el paso 4) amina-Ti-MOFs
6. Comparación de los resultados teóricos con los trabajos experimentales de nuestro grupo FuniMAT (www.icmol.es/funimat).

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Neyvis Almora Barrios

ACADEMIC TUTOR 2 Alechania Misturini Morelli

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física / Química Inorgánica

TITLE (Mandatory in English)

"Tuning Electronic and Optical Properties of Heterometallic Titanium Clusters Using Computational Tools"

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

1. Identificar los nodos heterometalicos de titanio (Ti) que existen en redes metal-orgánicas.

2. Emplear cálculos teóricos para comprender y predecir cómo los cambios en la composición y estructura de los nodos heterometálicos de Ti afectan sus propiedades electrónicas y ópticas.

3. Evaluar cómo las modificaciones estructurales y composicionales en los nodos de Ti influyen en sus propiedades ópticas.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. Revisión bibliográfica sobre los nodos heterometálicos de Titanio (Ti) en redes metal-organicas.
2. Construir modelos computacionales precisos de los nodos heterometálicos de Ti con diferentes composiciones y estructuras (segun el paso 1) . Se usaran programas de visualización de estructuras tales como GaussView, Materials Studio, Gdis, y VESTA.
3. Utilizar software de simulación avanzada como VASP (Vienna Ab-initio Simulation Package) y Gaussian, que permiten realizar cálculos de teoría del funcional de la densidad (DFT).
5. Investigar cómo las variaciones estructurales (como la sustitución de elementos) afectan las propiedades ópticas.
6. Comparar los resultados obtenidos mediante simulaciones con datos experimentales disponibles en la literatura científica.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Antonio Francés Monerris

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Theoretical study of the photophysics of Ru(II) transition metal complexes for photoinduced anticancer therapy

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The main goal of the study is to rationalize the absorption properties of Ru(II) complexes of interest in modern photodynamic therapy. The elucidation of the electronic structutre of the excited state provides relevant information such as the region of the molecule that participates in the excitation and the molecular properties of the excited state.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry and Inorganic Chemistry. The subject Computational Chemistry is strongly advised. Quantum chemistry software will be used to determine the nature, energies, and probabilities, among other properties, of the excited states of interest.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Carlos Bartual Murgui

ACADEMIC TUTOR 2 Teresa Delgado Pérez

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Departamento de Química Física

TITLE (Mandatory in English)

Syntesis and Characterization of New Iron(II) Spin Crossover Coordination Polymers

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Este trabajo tiene como objetivo introducir al estudiante en la transición de espín en compuestos de hierro(II), mediante la síntesis y caracterización de nuevos polímeros de coordinación 2D con ligandos -aceptores. Se busca desarrollar materiales multifuncionales que combinen propiedades como transición de espín, fluorescencia, porosidad o comportamiento huésped-anfitrión, con aplicaciones potenciales en sensores o materiales inteligentes.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

El trabajo comenzará con una revisión bibliográfica mediante el uso de bases de datos científicas accesibles desde la UV. A continuación, se llevará a cabo la síntesis de ligandos y complejos metálicos mediante técnicas de química orgánica y métodos de difusión lenta líquido-líquido. Los compuestos obtenidos se caracterizarán mediante espectroscopía IR, difracción de rayos X (monocristalina y en polvo), análisis termogravimétrico (TGA), medidas de adsorción (isotermas) y determinación de la susceptibilidad magnética.

Annex 1 (not to be printed)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Teresa Delgado Pérez

ACADEMIC TUTOR 2 Carlos Bartual Murgui

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Spin-crossover complexes as innovative contrast agents for magnetic resonance imaging (MRI)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- To review the fundamental principles of the spin-crossover (SCO) phenomenon and its impact on the magnetic properties of coordination complexes.
- To evaluate the current state of the art in the development of switchable SCO materials as smart, stimuli-responsive contrast agents for MRI.
-To analyze how the temperature- or light-induced transition between high-spin and low-spin states modulates water proton relaxation rates.
-To identify the main challenges regarding the biocompatibility, stability, and efficiency of these complexes for biomedical diagnostics.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Literature search: A comprehensive and systematic bibliographic search will be performed using high-impact scientific databases, primarily PubMed, Scopus, and Web of Science.

- Keywords selection: The search strategy will combine specific terms such as "spin crossover", "magnetic resonance imaging", "contrast agent", "relaxivity", and "iron(II) complexes".

-Data analysis and synthesis: The collected papers will be screened, classified, and critically analyzed. The student will organize the information into a monograph covering the synthesis, magnetic characterization, and biomedical performance of SCO-based MRI agents, concluding with a critical overview of future clinical perspectives.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Teresa Delgado Pérez

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Exotic and emerging applications of persistent luminescence materials

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- To explore the physical mechanisms of long-lasting phosphorescence (afterglow) and the design of advanced persistent luminescence materials.
- To compile and categorize "exotic" and non-conventional applications of these materials in fields such as anti-counterfeiting, optical information storage, forensics, and photocatalysis.
-To analyze the performance and advantages of persistent luminescence nanoparticles over conventional fluorescent markers in these emerging technological areas.
-To discuss the current limitations and future trends in the engineering of these smart materials for high-security and industrial applications.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Literature search: The student will conduct an extensive bibliographic review across multidisciplinary databases including Scopus, Web of Science, and Google Scholar to gather recent peer-reviewed articles.

- Keywords selection: Search queries will involve keywords such as "persistent luminescence", "afterglow nanoparticles", "anti-counterfeiting", "optical storage", "forensic science", and "stress sensing".

-Data analysis and synthesis: The student will screen the literature, extract relevant case studies of novel applications, and synthesize the data. The final report will be structured as a comprehensive review evaluating how these "exotic" properties are revolutionizing security technologies and advanced sensing, providing a clear map of the current state of the art.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Lourdes Gracia Edo

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Study of the selective oxidation over vanadia supported catalyst

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Study of the catalytically active site of vanadium oxide in three supported catalysts (SiO_2, TiO_2, ZrO_2).
- Study of the alcohol adsorption stage, preferably through the V-O-M junction (M = Si, Ti, Zr).
- Study of the stage of hydrogen transfer from the species $V\text{-}OCH_2CH_3$ to an O atom associated with the active center.
- Comparison of activation energy and rate coefficients for the three supported models.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The chemical reactivity of supported vanadium oxides has received considerable attention due to its importance in oxidation catalysis.

The GAUSSIAN program will be used to optimize all stationary points and to perform the corresponding vibrational analysis. Calculations based on Density Functional Theory (DFT) will be performed using appropriate functionals and basis sets to describe the atoms.

The intrinsic reaction coordinate method will be carried out to describe the paths of minimum energy that connect the transition structures with the corresponding minima.

Suggestion: to have taken the subject of Computational Chemistry

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Maria Carmen Martínez Bisbal

ACADEMIC TUTOR 2 Salvador José Cardona Serra

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Departamento de Química Física

TITLE (Mandatory in English)

Implementation of low-field NMR metabolomics for the determination of neurochemical brain alterations.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Prepare artificial solutions of the neurochemical biomarkers
Optimize acquisition parameters.
Compare spectra obtained at 80 MHz and 600 MHz.
Identify detectable neurochemical markers.
Develop multivariate statistical models.
Evaluate diagnostic potential.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Artificial solutions containing neurochemically relevant metabolites will be prepared to simulate simplified brain metabolomic profiles. The selected compounds will include representative brain metabolites such as N-acetylaspartate (NAA), glutamate, γ-aminobutyric acid (GABA), creatine, choline and myo-inositol among others. 1H-NMR spectra will be acquired using both a high-field spectrometer (600 MHz) and a benchtop low-field spectrometer (80 MHz), with the high-field spectra serving as the reference for metabolite assignment and spectral interpretation.
Spectral data will be processed using standard metabolomic workflows. The analytical performance of low-field NMR will be evaluated by performing spectra simulation using a Machine-learning procedure. Finally, multivariate statistical methods, will be employed to evaluate the ability of low-field NMR metabolomics to distinguish between different artificial neurochemical profiles and to assess its potential as a reliable platform for neurochemical metabolomic studies.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Mario Culebras Rubio

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Thermogalvanic cells based on microfluidic circuits

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Development of hydrogel precursors for microfluidic applications
Characterization of the rheological properties of the hydrogel precursors
Optimization of the redox couple concentration in the fluids
Assessment of the thermogalvanic performance of the microfluidic circuits

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Preparation of hydrogel precursors by varying the composition and polymer concentration to obtain suitable rheological properties for processing in microfluidic chips. Characterization of the rheological properties of the developed fluids by rheological measurements, including viscosity and shear-thinning behaviour. Evaluation of different redox couple concentrations to maximize the thermogalvanic performance of the fluids. Determination of the thermopower, output voltage, and power generation of the microfluidic thermogalvanic circuits under applied temperature gradients.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Mario Culebras Rubio

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Lignin-based hydrogels for thermogalvanic cells

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Synthesis of lignin-derived hydrogels
Morphological and structural characterization of the synthesized hydrogels
Optimization of the redox couple concentration
Evaluation of the thermogalvanic properties of the developed hydrogels

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Preparation of lignin-based hydrogels by varying the composition and crosslinking conditions in combination with other hydrophilic polymers
Characterization of the hydrogels using SEM, FTIR, TGA.
Evaluation of different redox couple concentrations to maximize thermogalvanic performance.
Determination of the thermopower, ionic conductivity, and output performance under applied temperature gradients.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 CRISTINA ROLDAN CARMONA

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): QUIMICA FÍSICA

TITLE (Mandatory in English)

Effect of seed layers on the photoluminescent efficiency of metal halide perovskites

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

MOED group (https://moed.es) has been a pioneer in Spain in the use of high-efficiency, hybrid vacuum-deposited perovskites for photovoltaics. This project aims to develop efficient optoelectronic devices by investigating the use of seed layers as growth templates for vacuum-deposited metal halide perovskite semiconductors. Special emphasis will be placed on how these layers influence crystallization dynamics and photoluminescence efficiency, with the goal of optimizing film quality and light-emission performance—key parameters in both photovoltaic technologies.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1) Fabrication of metal halide perovskite semiconductors using scalable vacuum deposition techniques.

2) Baseline optical and electrical characterization of the films and corresponding photovoltaic devices.

3) Integration of organic and inorganic seed layers to guide crystallization and interface formation.

4) Investigation of photophysical processes related to film quality and photoluminescence efficiency.

5) Optimization of solar cell performance.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 CLARA MARÍA GÓMEZ CLARI

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): PHYSICAL CHEMISTRY

TITLE (Mandatory in English)

Synthesis of thermoplastic polyurethanes with improved thermal resistance

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of this project is to obtain thermoplastic polyurethanes with improved thermal resistance by adding a selected additive. The thermal and mechanical properties of the obtained polyurethanes will be determined as a function of the content of additive.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The project is experimental as it involves the synthesis and chemical-physical characterization of thermoplastic polyurethanes modified by additives to improve the thermal resistance.
The student will synthesize different polyurethanes based on polycarbonate diol as a macrodiol, controlling the proportions of the rigid segment. Plates will be obtained for chemical-physical characterization. Thermal characterization will be performed using differential scanning calorimetry and thermogravimetric analysis, also molecular mass determination, and mechanical characterization of tensile and abrasion resistance properties will allow to asses the influence on thermal resistance of the additive.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 CLARA MARÍA GÓMEZ CLARI

ACADEMIC TUTOR 2 MARIO CULEBRAS RUBIO

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): PHYSICAL CHEMISTRY

TITLE (Mandatory in English)

Lignin/Cu2S Composites for Thermoelectric 3D-Printing Materials

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of the project is to synthesize and characterize Cu2S by different methods. These particles will be mixed with lignin to obtain materials with thermoelectric properties to be used in 3D printers. The thermoelectric properties of the materials will be characterized.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The project is experimental, as it involves the synthesis and chemical-physical characterization of Cu2S particles and lignin-Cu2S blends.
The student will synthesize different Cu2S particles controlling the structure to obtain good thermoelectric properties. Different porportions of Cu2S will be blended with lignin and other thermoplastic polymers to obtain inks for thermoelectric 3D materials. The physico chemical properties as well as the themoelectric properties will be characterized. 3D printing materials will be obtained and used to print a thermoelectric device. The thermolectric efficiency will be determined.

Annex I

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Daniel Roca Sanjuán

ACADEMIC TUTOR (if needed): Antonio Francés Monerris

EXTERNAL TUTOR (if needed):

Department: Química Física

TITLE (Mandatory in English)

Solar absorption spectra of atmospheric mercury compounds in water droplets

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Atmospheric mercurcy compounds absorb solar raditiation and this induces chemical processes which increase the lifetime of this compounds in the atmosphere and spread them over the planet. This knowledge is acquired from the properties of the compounds in the gas phase. However, the spectroscopical and chemical properties in clouds or humidity conditions have not been determined so far while they might have important implications on the atmospheric transport and planetary distribution of mercury. Our goul with this project will be to use the computational chemistry tools of the Quantum Chemistry of The Excited Sate group to predict the absorption spectra of the mercury compounds at the water-gas interface of water droplets where such species are known to be thermodynamically stable.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry II and III and Computational Chemistry, or in the Double Degree of Chemistry and Physics in the subject Elements of Physical Chemistry. Quantum chemistry calculations will be done to determine the vertical excitation energies and associated oscillator strengths and subsequently the spectra in mercury compounds equilibrated at the gas-water interface of water droplets.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Daniel Roca Sanjuán

ACADEMIC TUTOR (if needed): Antonio Francés Monerris

EXTERNAL TUTOR (if needed):

Department: Química Física

TITLE (Mandatory in English)

Molecular basis of the chemiluminescence-induced photodynamic therapy

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Photodynamics therapy is a technique used in biomedicine to treat certain types of solid tumors, infections or skin diseases. It is based on the administration of a drug that is activated by light irradiation of the ill tissue causing photodamage and destroying the pathological cells. One important limitation of the technique is that light cannot penetrate enough to destroy large and voluminous tumors. In this context, we are looking for a new generation of "autonomous" agents that deploy photoinduced antiproliferative activity without necessitating light absorption. Dioxetanes are of interest here because they produce excited states by thermal reactions and can activate the drugs used in PDT withouth the need of light. Our goal in this research project is to study the chemical process in which selected dioxetanes produces excited states without light.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry II and III and Computational Chemistry, or in the Double Degree of Chemistry and Physics in the subject Elements of Physical Chemistry. Quantum chemistry calculations will be done to determine reaction energy profiles for the chemical excitation of selected dioxetanes. Both multiconfigurational quantum chemistry and density functional theory will be considered for the study.

(Department stamp)

Annex I

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Daniel Roca Sanjuán

ACADEMIC TUTOR (if needed): Javier Segarra Martí

EXTERNAL TUTOR (if needed):

Department: Química Física

TITLE (Mandatory in English)

Free energies of cations and anions of nucleobases in DNA: A computational study

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

The ionization potentials and electron affinities of DNA nucleobases in the gas phase and aqueous solution is well determined both experimentally and theoretically. However, in the environment of nucleic acids, such property is not well known despite its relevance to understand the role of nucleobase cations and anions in the physiological conditions.

In this proposal, the student will use statistical thermochemistry and quantum chemistry to determine the free energies of the cations and anions of nucleobases with respect to the neutral systems in the DNA environment. The implications for the biological functions of nucleic acids will be also discussed.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry II and III and Computational Chemistry, or in the Double Degree of Chemistry and Physics in the subject Elements of Physical Chemistry. Hybrid methods combining quantum and classical mechanics will be used. Molecular dynamics simulations will be also performed to obtain the free energy change in the process of transforming a neutral nucleobase into a cation or anion in the DNA environment.

(Department stamp)

Annex I

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Daniel Roca Sanjuán

ACADEMIC TUTOR (if needed): Antonio Francés Monerris

EXTERNAL TUTOR (if needed):

Department: Química Física

TITLE (Mandatory in English)

Oxidation potential of DNA quadruplexes

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Guanine quadruplexes are regions in nucleic acids in which oxidation maybe facilitated. However, the oxidation potential remains to be determined with accuracy. In this proposal, the student will use statistical thermochemistry and quantum chemistry to determine the free energies of the guanine cations formed in such regions and will discuss the implications that the findings might have in DNA charge transport.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry II and III and Computational Chemistry, or in the Double Degree of Chemistry and Physics in the subject Elements of Physical Chemistry. Hybrid methods combining quantum and classical mechanics will be used. Molecular dynamics simulations with appropriate force fields will be carried out to obtain equilibrated structures of guanine quadruplexes. Next, the free energy change in the process of transforming a neutral nucleobase into a cation will be computed by means of free-energy perturbation techniques.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Kirill Zinovjev

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Validation of AI-predicted conformational ensembles of disordered peptides

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Long molecular dynamics (MD) simulations will sample the conformational ensembles of a set of short disordered peptides (chosen with the student) and be compared with the ensembles generated by AlphaFold2 (AF2).
Specific objectives:
- Select the peptides and prepare the simulation systems
- Sample their conformational space by long MD simulations
- Generate structural ensembles with AlphaFold2
- Test whether AF2 recovers the most populated states and their populations

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Molecular Dynamics (Amber)
Structure prediction (AlphaFold2)
Trajectory analysis and clustering (Python, MDAnalysis)
Data Analysis (Python)

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Muñoz-Espí

ACADEMIC TUTOR 2 Mario Culebras Rubio

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Colloidal Encapsulation of High-Temperature Phase Change Materials

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- To develop encapsulation strategies for high-temperature phase change materials (PCMs).
- To prepare encapsulated inorganic PCMs using colloidal methods.
- To characterize the morphology and thermal properties of the prepared materials.
- To evaluate their potential for thermal energy storage applications.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The methodology to be used will involve:

1. The use of nanostructuring techniques based on "soft templating" methods.
2. Thermal analysis using differential scanning calorimetry (DSC) and thermogravimetry (TGA).
3. Morphological analysis using scanning and transmission electron microscopy (SEM/TEM).
4. Structural analysis using infrared spectroscopy (FTIR).
5. Evaluation of the applicability of the materials in thermal energy storage.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Iñaki Tuñón

ACADEMIC TUTOR 2 Jose Javier Ruiz

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

A Computational Approach to the Study of Enzymatic Mechanisms.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Construcción de un modelo representativo del centro activo de la enzima en estudio.
Optimización del modelo reducido de una conformación o estructura de rayos X de la enzima.
Estudio del mecanismo de reacción de la enzima en presencia del sustrato natural, estableciendo las diferentes etapas y las barreras de energía potencial.
Determinación de las barreras de energía libre.
Comparación de las propiedades cinéticas y termodinámicas del modelo construido con los datos experimentales disponibles.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se utilizarán métodos de cálculo de Química Cuántica.
El estudio se realizará utilizando fundamentalmente el programa Gaussian, con posibilidad de utilización de ORCA. Además se usarán programas de visualización de estructuras, tal como: Molden, Gaussview o VMD.
Localización de los puntos estacionarios asociados al proceso catalítico.
Determinación de la constante de velocidad para cada uno de las etapas de la reacción analizadas.
Determinación de la constante de equilibrio del sistema y evaluación respecto a valores determinados experimentalmente.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Álvaro Martínez Camarena

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Insights into the recognition of neurotransmitters by azamacrocycles: A theoretical approach.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Caracterització estructural i energètica de la interacció lligand-neurotransmissor en fase gas.
- Estudi de l'efecte del solvent i dinàmica del reconeixement molecular en solució aquosa.
- Determinació del perfil termodinàmic i de la selectivitat del reconeixement

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

L'estudi del reconeixement molecular de neurotransmissors per receptors sintètics és fonamental per al desenvolupament de nous sensors biomèdics i agents terapèutics. En este treball es busca analitzar les subtils forces intermolèculars que governen la selectivitat cap a dianes d'alt impacte biològic com la serotonina, la dopamina i la tirosina. Per a abordar aquest repte, s'emprarà una metodologia computacional multiescala combinada: la mecànica quàntica (QM), basada en la teoria del funcional de la densitat (DFT), proporcionarà una descripció precisa de la geometria i l'energia de lligand dels complexos en fase gas, mentre que les simulacions de dinàmica molecular (MD) permetran avaluar l'estabilitat conformacional i el perfil termodinàmic dels sistemes en un entorn aquós realista. Amb este enfocament, l'estudiant adquirirà competències clau en química física teòrica amb aplicació directa en el disseny racional de receptors supramoleculars.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Francisco F. Pérez Pla

ACADEMIC TUTOR 2 M. Ángeles Úbeda Picot

EXTERNAL TUTOR (if needed): --

DEPARTMENT(S): Química Física y Química Inorgánica

TITLE (Mandatory in English)

Design, Preparation and Catalytic Performance of Sustainable Nickel Nanoparticles Supported on Carbonized Polydopamine/magnetite cores.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of this study is to synthesize carbon-coated core-shell magnetite microparticles that serve as an environmentally friendly support for Ni nanoparticles. Throughout this final-year project, the structural characterization of the prepared material will be carried out using various techniques, including ICP, TGA, TEM, EDX-SEM, FTIR, and Raman. Following the characterization, the catalytic activity and stability of the prepared material will be evaluated in relation to the reduction of nitrobenzene to aniline, a reaction of both environmental and industrial importance.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The particles will be prepared by polymerizing dopamine on the surface of Fe3O4 microcrystals. This support will be impregnated with cations of Ni(II), which will subsequently be reduced by pyrolysis in a controlled N2 atmosphere. This methodology allows for the preparation of structured "core-shell" compounds. Following synthesis, the materials will undergo characterization using thermogravimetric analysis. The specific surface area and porosity will be determined using nitrogen adsorption isotherms. A morphological analysis of the particles will be performed using transmission electron microscopy. The Ni(II) deposited will be analyzed using scanning electron spectroscopy, and the nature of the carbon layer will be evaluated using Raman spectroscopy. Finally, the material's catalytic activity will be evaluated in terms of the reduction of nitrobenzene to aniline using DAD-UV-Vis absorption measurements and HPLC.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Muñoz-Espí

ACADEMIC TUTOR 2 Francisco F. Pérez Pla

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Application of Functionalized Polymer Nanoparticles in Asymmetric Catalysis

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Preparation of polymer nanoparticles functionalized with organic or organometallic moieties, with ability to catalyze asymmetrically organic reactions.

- Evaluation of the catalytic activity of the prepared materials.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The catalytic moieties will be supported on polymer nanoparticles prepared by colloidal methods (typically, miniemulsion polymerization). The colloidal characterization of the systems will be performed using dynamic light scattering (DLS) and zeta potential measurement. The morphology of the materials will be evaluated using electron microscopy (SEM and TEM). Thermogravimetric analysis (TGA) will be used for thermal characterization.

The catalytic activity and the stereoselectivity will be studied by using liquid chromatography (HPLC).

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jose Javier Ruiz

ACADEMIC TUTOR 2 Iñaki Tuñón

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Characterization of Enzyme Catalytic Properties Using Molecular Dynamics Simulations.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Análisis del espacio conformacional de la proteína en estudio.
Determinación de los parámetros energéticos y geométricos más relevantes que permitan entender el comportamiento del sistema en estudio.
Determinación de poblaciones conformacionales y sus probabilidades mediante análisis de componentes principales.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se utilizarán métodos de cálculo de simulación computacional.
El estudio se realizará utilizando fundamentalmente el programa AMBER y AMBERTOOLS.
Además se usarán programas de visualización de estructuras, tal como VMD, PYMOL, etc.
Programas de análisis en PYTHON. Implementación de scripts en la plataforma Júpiter.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Mario Culebras Rubio

ACADEMIC TUTOR 2 Francisco F. Pérez Pla

EXTERNAL TUTOR (if needed): --

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Transforming Biomass into Advanced Electrocatalysts: Pyrolyzed Lignin–Metal Electrodes for Green Aromatic Nitro Compound Reduction

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The main objective of this final-year project is to develop a new generation of sustainable electrocatalytic electrodes based on pyrolyzed lignin impregnated with earth-abundant transition metals for the selective electrochemical reduction of nitrobenzene to aniline under environmentally benign conditions. To achieve this goal, the project will optimize the preparation of lignin-derived carbon coatings on inert conductive substrates, investigate the influence of metal incorporation and controlled pyrolysis on the structural, physicochemical, and electrochemical properties of the resulting materials, and establish clear structure–activity relationships governing catalytic performance. Special attention will be devoted to maximizing catalytic activity, selectivity, stability, and Faradaic efficiency while minimizing competing hydrogen evolution.
Ultimately, the project aims to demonstrate that renewable lignin can be transformed into high-performance electrocatalysts, providing an efficient and cost-effective alternative to noble-metal-based electrodes for the sustainable electrosynthesis of aromatic amines.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The final-year project will follow an integrated methodology combining materials synthesis, advanced physicochemical characterization, and electrochemical evaluation. Thin lignin coatings will be deposited onto inert conductive substrates and subsequently impregnated with aqueous solutions of 3d cation salts to promote homogeneous metal coordination within the biopolymer matrix. The resulting precursors will be subjected to controlled pyrolysis under inert atmosphere to produce metal–carbon composite electrodes with tailored structural and electronic properties. The influence of the metal precursor, metal loading, pyrolysis temperature, and processing conditions on the morphology, porosity, graphitization degree, surface chemistry, and metal dispersion will be systematically investigated using complementary techniques such as SEM, TEM, XRD, Raman spectroscopy, XPS, BET surface area analysis, and ICP-OES. The electrocatalytic performance of the prepared electrodes toward nitrobenzene reduction will be assessed by cyclic voltammetry, linear sweep voltammetry, chronoamperometry, electrochemical impedance spectroscopy, and product analysis by chromatographic and spectroscopic methods. Correlating catalyst structure with electrochemical activity, selectivity, Faradaic efficiency, and long-term stability will enable the identification of the key physicochemical parameters governing catalytic performance and provide design principles for the development of efficient, sustainable lignin-derived electrocatalysts.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Muñoz-Espí

ACADEMIC TUTOR 2 Francisco F. Pérez Pla

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Polysaccharide-Based Hybrid Particles as Magnetically Separable Catalysts

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Preparation of polysaccharide particles for complexation of metal ions, so that the can be used in model catalytic reactions.

- Evaluation of the catalytic activity of the prepared materials.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The preparation of the macroscopic particles will take place by ionotropic gelation according to the methods previoulsy developed in our laboratory. Magnetite nanoparticles will be integrated in the system.

Metal ions will be incorporated into the systems either in situ during the preparation of the particles or by post-loading. The metal ions can be reduced to obtain metallic particles on the surface of the particles.

The catalytic activity will be evaluated by UV-vis spectroscopy and/or by chromatography.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Francisco F. Pérez Pla

ACADEMIC TUTOR 2 M. Ángeles Úbeda Picot

EXTERNAL TUTOR (if needed): --

DEPARTMENT(S): Química Física y Química Inorgánica.

TITLE (Mandatory in English)

From Sustainable Materials to Efficient Catalysts: Preparation and Evaluation of Cobalt Nanoparticles on Carbonized Polydopamine/Co3O4 magnetic cores.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of this study is to synthesize a carbon-based "core-shell" composite material containing cobalt ferrite (C@Co3O4) to serve as an environmentally friendly support for biometals. During the final-year project, the structural characterization of the prepared material will be carried out using various techniques: ICP, TGA, EDX-SEM, TEM, BET, and Raman. The second task of the project will consist of evaluating the material's catalytic activity and stability in relation to the reduction of nitrobenzene to aniline using HPLC. This is a reaction of both environmental and industrial importance.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The particles will be prepared by polymerizing dopamine on the surface of Co_3O_4 micro/nanocrystals. This support will be impregnated with cations of the biometal, which will subsequently be reduced by carbonization in a controlled N2 atmosphere. This methodology allows for the preparation of structured "core-shell" compounds. Following synthesis, the materials will undergo characterization using thermogravimetric analysis. The specific surface area and porosity will be determined from nitrogen adsorption isotherms, and a morphological analysis of the particles will be performed using transmission electron microscopy. The biometal deposited will be analyzed using scanning electron spectroscopy, and the nature of the carbon layer will be evaluated using Raman spectroscopy. Finally, the material's catalytic activity will be evaluated in terms of the reduction of nitrobenzene to aniline using DAD-UV-Vis absorption measurements and HPLC.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 José Juan García Jareño

ACADEMIC TUTOR 2 Jerónimo Agrisuelas Vallés

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

Color in the Chemistry Laboratory: Theoretical Foundations, Quantitative Rigor, and Instrumental Development.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

General Objective:
To systemize and critically analyze the theoretical foundations, quantitative control methods, and instrumental innovations regarding the use and measurement of color within the modern chemistry laboratory, evaluating its evolution from visual perception to current digital instrumentation.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

This bibliographical research will follow a systematic approach across four main stages. First, a comprehensive literature search will be conducted in databases like Scopus and ScienceDirect using keywords related to colorimetry, digital imaging, and low-cost sensing. Retrieved papers will be selected based on strict quality criteria and categorized into theoretical, algorithmic, and instrumental frameworks.
Data extraction will focus on comparing key analytical parameters—such as precision, limits of detection, and calibration strategies—against classical spectrophotometry.
Finally, the synthesized data will be critically evaluated to identify research gaps and future trends in laboratory automation.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Javier Segarra Martí

ACADEMIC TUTOR 2 Lewis Hutton

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Microsolvation effects on the photophysical reactivity of DNA model systems

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- To understand how microsolvation affects the UV-Vis radiation absorption in DNA/RNA chromophores and the ensuing reactivity, which is key to rationalising their photostability.
- To introduce the student to the field of computational chemistry, particularly to the simulation of electronic excited states and their interpretation, including spectroscopy and reactivity.
- To gain data handling competencies, including parsing and curating data using basic programming tools like Python.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

DNA/RNA nucleobases (Ade, Cyt, Thy, Ura, and Gua) encode our genetic material and are key to life. However, exposure to UV-Vis radiation has been linked with deleterious societal concerns like skin cancer/melanoma. While the effects of UV-Vis radiation on our genetic lexicon are well understood in the gas phase, it remains unclear how the biological media in which DNA is embedded affects the photophysics of the nucleobases. This project proposes modelling simple DNA/RNA systems under different microsolvation conditions to understand how specific solvent positioning may affect reactivity, and whether a systematic increase in microsolvation can bridge the gap with the photo-properties in the condensed phase. To do this, the following plan will be followed:

1) In-depth search of the literature for the different models and experiments available.
2) Modelling the UV-Vis absorption spectrum and excited state relaxation pathways of selected microsolvated DNA/RNA species.
3) Analyse the results obtained and contrast them against results found in the literature.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR 2 José Juan García Jareño

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

Separation of cobalt and nickel metals by selective electrodeposition on different types of electrodes.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To evaluate the selective electrodeposition kinetics of cobalt and nickel mixtures on different electrode materials by voltammetric analysis.

To optimize operational parameters—such as applied potential, pH, and electrolyte composition—to maximize separation efficiency and purity.

To characterize the composition and surface morphology of the electrodeposited metallic phases to verify successful separation.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Literature Search: Review databases like Scopus or WOS for selective Co/Ni electrodeposition and electrode substrate performance.

Experimental Assay: Perform voltammetric screening and controlled-potential electrolysis to determine optimal separation conditions.

Characterization: Analyze the composition, purity, and morphology of the electrodeposited metallic phases.

Report Writing: Process experimental data, benchmark findings against literature, and draft the final manuscript.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR 2 José Juan García Jareño

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

Mineralization of water pollutants by advanced oxidation techniques and spectroelectrochemical monitoring.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Use of reusable electrodes for electrochemical removal of pollutants.
Approach to the study of advanced oxidation processes.
Optimization and monitoring of the process by spectroelectrochemical techniques.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. Bibliographic study
2. Introduction to the electrochemical techniques.
3. Electrode preparation.
4. Design of electrochemical experiments.
5. Analysis of obtained results and discussion.
6. Writing the TFG report.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR 2 José Juan García Jareño

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

Generation of reactive oxygen species (ROS) on steel/poly(phenothiazines) electrodes and their application.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To synthesize steel/poly(phenothiazines) electrodes and characterize their physicochemical and electrochemical properties.

To quantify the generation efficiency of reactive oxygen species (ROS) produced on the modified electrode surfaces.

To evaluate the application of these ROS-generating electrodes in a target process, such as pollutant degradation or disinfection.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Literature Review.
Electrode Preparation: Synthesize poly(phenothiazines) films electrochemically onto steel substrates under optimized deposition conditions.
Characterization: Analyze the modified electrodes using cyclic voltammetry, impedance spectroscopy, and surface characterization techniques.
ROS Monitoring: Detect and quantify the generated reactive oxygen species using specific chemical probes and spectroscopic methods.
Application Testing: Evaluate the performance of the electrodes in degradation or disinfection assays under controlled electrochemical operation.
Data Analysis: Correlate polymerization parameters and ROS generation efficiency to optimize the system's analytical or environmental performance.
Write the Degree Final Project report.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR 2 José Juan García Jareño

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

Electroplating of copper on composite materials of the screen printed carbon electrodes for their possible use in sensors.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To optimize the electrochemical deposition parameters for electroplating copper onto screen-printed carbon electrodes (SPCEs) modified with composite materials.
To characterize the morphology, surface structure, and electrochemical properties of the resulting Cu-modified composite electrodes.
To evaluate the electrocatalytic activity and analytical performance of the developed sensors toward a target analyte.
To assess the reproducibility, stability, and operational lifetime of the copper-electroplated composite platforms for sensor applications.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Literature Review.
Substrate Modification: Prepare the screen-printed carbon electrodes (SPCEs) with the target composite materials to serve as the conductive base.
Copper Electroplating: Perform electrochemical deposition of copper onto the composite-modified SPCEs under optimized current and time conditions.
Physicochemical Characterization: Analyze the surface morphology, composition, and electrochemical behavior of the Cu-composite platforms using voltammetry and microscopy.
Sensor Performance Testing: Evaluate the analytical response, sensitivity, and stability of the developed sensors toward the target analyte.
Write the report.

Annex I

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Daniel Roca Sanjuán

ACADEMIC TUTOR (if needed): David Francisco Macias Pinilla

EXTERNAL TUTOR (if needed):

Department: Química Física

TITLE (Mandatory in English)

Revisiting the absorption cross sections of atmospheric mercury compounds with anharmonic corrections and probabilistic machine learning

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Atmospheric mercury compounds absorb solar raditiation and this induces chemical processes which increase the lifetime of this compounds in the atmosphere and spread them over the planet. This knowledge is acquired from the inclusion of computed absorption cross sections in climate models. In the last 5 years, the Quantum Chemistry of The Excited Sate group has developed new tools, implemented in our MultiSpec software, to improve the computational determination of such properties including anharmonic corrections to describe the quantum vibrations of nuclei and probabilistic machine learning to minimize the statistical errors. In this research projects, our goal is to recompute the absorption cross sections of the mercury compounds with such new tools and discuss on the implications that it may have in the atmospheric transportation and distribution of mercury.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry II and III and Computational Chemistry, or in the Double Degree of Chemistry and Physics in the subject Elements of Physical Chemistry. Quantum chemistry calculations will be done to determine the vertical excitation energies and associated oscillator strengths and subsequently the spectra in mercury compounds. The MultiSpec platform that the group has developed will be used for the computations including the anharmonic corrections and probabilistic machine learning.

(Department stamp)

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Javier Segarra Martí

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Modelling the water UV/Vis spectrum: from gas phase to liquid

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- To provide a molecular mechanism behind the UV/Vis spectral shift observed experimentally in water through the modelling of clusters of increasing size and complexity, establishing a clear link between hydrogen-bonding coordination and absorption.
- To introduce the student to the field of computational chemistry, particularly to the simulation of electronic excited states and their interpretation, including spectroscopy and reactivity.
- To acquire essential digital data handling competencies, including parsing and curating data using simple programming tools/languages like Python.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Despite its importance as the most relevant substance to life, water remains relatively misunderstood as it features anomalies across most of its properties according to its chemical composition: its boiling/melting/critical point and viscosity are high, it shrinks on melting, has a high density that increases upon heating and has an increase in the hydrogen bonding coordination pattern with increased temperature (and on melting) amongst others. The project focusses on characterising the energy shift observed when going from gas phase to liquid in the registered UV/Vis spectrum, providing an as of yet missing molecular counterpart to rationalise it. To do so the student will:

1) In-depth search of the literature for the different models and experiments available.
2) Model the electronic excited states of a range of water clusters of increasing size and complexity, bridging the gap between the gas phase (single molecules infinitely separated) and liquid (crowded environments with different hydrogen-bonded coordination patterns).
3) Analyse the results obtained and contrast them against results found in the literature.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Joaquín Calbo Roig

ACADEMIC TUTOR 2 Enrique Ortí Guillén

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Department of Physical Chemistry

TITLE (Mandatory in English)

First-principles characterization of honeycomb 2D MOFs as porous conductors

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El objetivo principal de este trabajo es establecer relaciones de estructura–propiedad en una familia de redes metal-orgánicas (MOFs) bidimensionales con arquitectura tipo panal (honeycomb), explorando modificaciones químicas que permitan guiar el diseño racional de nuevos materiales porosos con conductividad eléctrica. En particular, se analizará el impacto de:

1. El metal de transición empleado como nodo inorgánico.
2. La naturaleza del grupo anclaje del ligando orgánico.
3. El grado de conjugación π del sistema molecular orgánico.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. Revisión bibliográfica sobre MOFs 2D de tipo honeycomb construidos a partir de ligandos basados en anillos de benceno, trifenileno y trinaftileno, caracterizados experimental o teóricamente en la literatura.
2. Optimización y análisis estructural de los sistemas cristalinos propuestos, mediante cálculos de tipo DFT (Density Functional Theory).
3. Análisis de estabilidad estructural, si procede, considerando configuraciones alternativas de apilamiento entre capas vecinas (autoensamblaje).
4. Caracterización teórica de las propiedades electrónicas mediante el cálculo de la estructura de bandas, densidad de estados, análisis de cargas y densidad de spin.
5. Evaluación de propiedades de transporte, mediante el cálculo de masas efectivas y/o acoplamientos electrónicos entre unidades electroactivas, como indicadores clave del comportamiento conductor.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jesús Vicente de Julián Ortiz

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed): Sofiane Benmetir

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Development and Evaluation of Immersive Virtual Reality and Augmented Reality Modules for Teaching Stereochemistry, Crystal Structures, and Protein Architecture.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Develop fully functional VR/AR interactive modules for visualizing stereochemistry, crystal unit cells, and protein structures.

Pilot-test these modules with a diverse group (students and educators) to evaluate usability, engagement, and learning effectiveness through observations, logs, and questionnaires.

Analyze collected data to iteratively refine the materials and formulate evidence-based recommendations for integrating VR/AR into chemistry education.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Define specific learning outcomes and develop high-fidelity 3D models and interactive tools (e.g., mirror tool, unit-cell builder) using Unity 3D and Blender, guided by initial storyboards.

Recruit a diverse pilot group to conduct hands-on testing sessions, collecting in-app usage metrics, observational notes, and structured feedback questionnaires.

Perform a mixed-methods analysis (qualitative thematic analysis and quantitative descriptive statistics) to identify usability and pedagogical gaps, leading to final iterative refinements.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jesús Vicente de Julian Ortiz

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed): Sofiane Benmetir

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Design of Rotavirus Inhibitor Compounds

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To design covalent inhibitors of the rotavirus receptor that binds to glycoproteins of intestinal epithelial cells.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Structure-based drug design techniques on the rotavirus binding domain.
Perform virtual screening of compound libraries (e.g., commercially available databases, in-house libraries) to identify potential inhibitors. Docking simulations will be used to assess the binding affinity and binding mode of candidate compounds to the receptor.
Validation of the inhibitors designed by using cell culture assay. Identify potential sources of discrepancies between simulations and experiments.
Design covalent inhibitors by incorporating electrophilic warheads into the identified candidate compounds. The warheads will be positioned to react with nucleophilic residues (e.g., lysine, serine, cysteine) within the binding site of the receptor.
Conduct molecular dynamics (MD) simulations to assess the stability and binding affinity of the designed covalent inhibitors.

Annex 1 (**not to be printed**)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jesús Vicente de Julián Ortiz

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed): Sofiane Benmetir

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Computational Simulation of the T-lymphocyte receptor

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To develop a model capable of simulating the behavior of membrane proteins within an electric field, accurately representing the electrostatic interactions and conformational changes.
To apply this model to simulate the molecular dynamics of the interaction between the T-lymphocyte receptor complex and the Major Histocompatibility Complex, focusing on the influence of electric fields on the conformation changes.
To analyze the simulation data to identify key residues and interactions that are significantly affected by the presence of electric fields.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

System Setup: To construct detailed atomistic models of the complexes using available structural data (e.g., PDB files). Embed these complexes within a realistic membrane environment using appropriate lipid molecules. Define the electric field parameters (magnitude, direction).
Molecular Dynamics Simulations: Employ state-of-the-art molecular dynamics (MD) simulation software (e.g., NAMD, GROMACS) with appropriate force fields (e.g., CHARMM, AMBER) to simulate the system's behavior under the influence of the electric field.
Data Analysis: Analyze the simulation trajectories to characterize the conformational dynamics of the proteins and the effects of the electric field. The applicability and usefulness of virtual reality techniques for visualizing these interactions will be studied.